

MDF: Magnetic Particle Imaging Data Format

T. Knopp^{1,2}, T. Viereck³, G. Bringout⁴, M. Ahlborg⁵, A. von Gladiss⁵, C. Kaethner⁵, P. Vogel⁶, J. Rahmer⁷, M. Möddel^{1,2}

¹Section for Biomedical Imaging, University Medical Center Hamburg-Eppendorf, Germany

²Institute for Biomedical Imaging, Hamburg University of Technology, Germany

³Institute of Electrical Measurement and Fundamental Electrical Engineering, TU Braunschweig, Germany

⁴Physikalisch-Technische Bundesanstalt, Berlin, Germany

⁵Institute of Medical Engineering, University of Lübeck, Germany

⁶Department of Experimental Physics 5 (Biophysics), University of Würzburg, Germany

⁷Philips GmbH Innovative Technologies, Research Laboratories, Hamburg, Germany

June 22, 2017

Version **2.0.0-pre**

Abstract

Magnetic particle imaging (MPI) is a tomographic method to determine the spatial distribution of magnetic nanoparticles. In this document a file format for the standardized storage of MPI and magnetic particle spectroscopy (MPS) data is introduced. The aim of the Magnetic Particle Imaging Data Format (MDF) is to provide a coherent way of exchanging MPI and MPS data acquired with different devices worldwide. The focus of the file format is on sequence parameters, measurement data, and reconstruction data. The format is based on the hierarchical document format (HDF) in version 5 (HDF5). This document discusses version 2 of the MDF, which is not backward compatible with version 1.

1 Prior to release: ToDo

- Update arXiv version and the corresponding entry in `MDF.bib`
- Move sanitycheck to `MPIFile.jl`
- mention `MPIFile.jl` written in the Julia programming language [1, 2, 3]

- Update Examples
- Update Changelog

2 Introduction

The purpose of this document is to introduce a file format for exchanging Magnetic Particle Imaging (MPI) and Magnetic Particle Spectroscopy (MPS) data. The Magnetic Particle Imaging Data Format (MDF) is based on the hierarchical document format (HDF) in version 5 (HDF5) [4]. HDF5 is able to store multiple datasets within a single file providing a powerful and flexible data container. To allow an easy exchange of MPI data, one has to specify a naming scheme within HDF5 files which is the purpose of this document. In order to create and access HDF5 data, an Open Source C library is available providing dynamic access from most programming languages. Matlab supports HDF5 by the functions `h5read` and `h5write`. For Python the `h5py` package exists. The Julia programming language provides access to HDF5 files via the `HDF5` package. For languages based on the .NET framework the `HDF5DotNet` library is available.

The MDF is mainly focused on storing measurement data, system matrices, or reconstruction data together with corresponding sequence parameters and metadata. Though it is possible to combine measurement data and reconstruction data into a single file it is recommended to use a single file for each of the following dataset types:

1. Measurement data
2. System calibration data
3. Reconstruction data

2.1 Datatypes

MPI parameters are stored as regular *HDF5 datasets*. *HDF5 attributes* are not used in the current specification of the MDF. For most datasets a fixed datatype is used, i.e. the drive-field amplitudes are

stored as `H5T_NATIVE_DOUBLE` values. For our convenience we refer to the HDF5 datatypes `H5T_STRING`, `H5T_NATIVE_DOUBLE` and `H5T_NATIVE_INT64` as `String`, `Float64` and `Int64`. Boolean data is stored as `H5T_NATIVE_INT8`, which we refer to as `Int8`.

The datatype of the measurement data and the calibration data offers more freedom and is denoted by `Number`, which can be any of the following HDF5 data types: `H5T_NATIVE_FLOAT`, `H5T_NATIVE_DOUBLE`, `H5T_NATIVE_INT8`, `H5T_NATIVE_INT16`, `H5T_NATIVE_INT32`, and `H5T_NATIVE_INT64`. The same holds true for the `Integer` data type, which can be any of: `H5T_NATIVE_INT8`, `H5T_NATIVE_INT16`, `H5T_NATIVE_INT32`, and `H5T_NATIVE_INT64`.

For later identification of a data set we store three UUIDs (RFC 4122) [5] in its canonical textual representation as 32 hexadecimal digits, displayed in five groups separated by hyphens 8-4-4-4-12 as for example `ee94cb6d-febf-47d9-bec9-e3afa59bfaf8`. For the generation of the UUIDs we recommend to use version 4.

Since storing complex data in HDF5 is not standardized, we extend the dimensionality of an existing array and store the real and imaginary part in the last dimension with size 2 (index 0 = real part, index 1 = imaginary part). In this way the real and imaginary part of a complex datum is stored sequentially on disk.

2.2 Units

Physical quantities are given in SI units with one exception. The field strength is reported in $\text{T}\mu_0^{-1} = 4\pi\text{Am}^{-1}\mu_0^{-1}$. This convention has been proposed in the first MPI publication [6] and since that time consistently used in most MPI related publications. The aims of this convention are to report the numbers on a Tesla scale, which most readers with a background in MRI are familiar with and use the correct unit for the magnetic field strength.

2.3 Optional Parameters

The MDF has 8 main groups in the root directory and 2 sub-groups. We distinguish between optional and non-optional groups and optional, non-optional, and conditional parameters. Any optional parameter can be omitted, whereas any non-optional parameter in a non-optional group is mandatory. Conditional parameters are linked to Boolean parameters and have to be provided if that parameter is true and can be omitted if that parameter is false. If a parameter is optional, non-optional, or conditional is indicated by yes, no, or the corresponding Boolean parameter respectively.

If a group is optional all of its parameters may be omitted if this group is not used. The groups `/`, `/study`, `/experiment`, `/scanner`, `/acquisition` contain mostly metadata and are mandatory. The `/tracer` group is only mandatory if magnetic material has been placed in the scanner. The groups `/measurement`, `/calibration`, and `/reconstruction` are all optional. `/measurement` is optional but MPI measurement data as well as calibration data will be stored here. In case of calibration measurements, the `/calibration` group is mandatory. Reconstruction data is stored in `/reconstruction`. One should not store regular measurements, calibration data, and reconstruction results in a single MDF. Instead, individual files should be used.

2.4 Parameter Extension

Often it is necessary to store additional specific parameters or metadata not covered in the specifications, like for example the temperature of the room in which your MPI device is operated. In this case you are free to add new parameters to any of the existing groups. Moreover if necessary you are also free to introduce new groups. To be able to distinguish these datasets and groups from the specified ones we recommend to use the prefix `_` for all parameters and groups. As an example one could add a new group `/_room` and within the dataset `_temperature`.

2.5 Naming Convention

Several parameters within an MDF are linked in the dimensionality. We use short variable names to indicate these connections. The following table describes the meaning of each used variable name

Variable	Meaning: Number of...
A	tracer materials/injections for multi-color MPI
N	acquired frames, same as a spatial position for calibration
O	acquired frames w/o background frames
J	focus-field patches
C	receive channels
D	drive-field channels
F	frequencies describing the drive-field waveform
U	sampling points describing a custom drive-field waveform
V	points sampled at receiver during one patch (product of drive field period , numPeriods , numAverages)
W	sampling points containing processed data ($W = V$ if no frequency selection or bandwidth reduction has been done)
K	frequencies describing processed data ($K = V/2 + 1$ if no frequency selection or bandwidth reduction has been done)
Q	frames in the reconstructed MPI data set
P	voxels in the reconstructed MPI data set
S	channels in the reconstructed MPI data set

2.6 Contact

If you find mistakes in this document or the specified file format or if you want to discuss extensions to this specification, please open an issue on GitHub:

<https://github.com/MagneticParticleImaging/MDF>

As the file format is versionized it will be possible to extend it for future needs of MPI. The current version discussed in this document is version 2.0.0-pre.

2.7 arXiv

As of version 1.0.1 the most recent release of these specifications can also be also found on the arXiv:

<https://arxiv.org/abs/1602.06072>

If you use MDF please cite us using the arXiv reference, which is also available for download as `MDF.bib` from GitHub.

2.8 Code examples

If you want to get a basic impression of how to handle MDF files you can visit the gitub repository of the MDF project:

<https://github.com/MagneticParticleImaging/MDF>

There you will find the directory example, which contains a code example written in Julia, Matlab and Python. More details can be found in the README of the repository.

3 Data (group: /)

Remarks: Within the root group metadata about the file itself is stored. Within several subgroups, metadata about the experimental setting, the MPI tracer, and the MPI scanner can be provided. The actual data is stored in dedicated groups on measurement data and reconstruction data.

Parameter	Type	Dim	Unit/Format	Optional	Description
version	String	1	2.0.0	no	Version of the file format
uuid	String	1	3170fdf8-f8e1-4cbf-ac73-41520b41f6ee	no	Universally Unique Identifier (RFC 4122) of MDF file
time	String	1	yyyy-mm-ddThh:mm:ss.ms	no	UTC creation time of MDF data set

3.1 Study Description (group: /study/, non-optional)

Remarks: A study is supposed to group a series of experiments to support, refute, or validate a hypothesis. The study group has to contain `name`, `number`, `uuid`, and `description` of the study.

Parameter	Type	Dim	Unit/Format	Optional	Description
name	String	1		no	Name of the study
number	Int64	1		no	Experiment number within study
uuid	String	1	295258fe-b650-4e5f-96db-b83f11089a6c	no	Universally Unique Identifier (RFC 4122) of study
description	String	1		no	Short description of the study

3.2 Experiment Description (group: /experiment/, non-optional)

Remarks: For each experiment within a study `name`, `number`, `uuid`, and `description` have to be provided. Additionally, the name of the imaged `subject` and a flag indicating if data has been obtained via simulations `isSimulation` has to be stored.

Parameter	Type	Dim	Unit/Format	Optional	Description
name	String	1		no	Experiment name
number	Int64	1		no	Experiment number
uuid	String	1	f96dbc48-1ebd-44c7-b04d-1b45da054693	no	Universally Unique Identifier (RFC 4122) of experiment
description	String	1		no	Short description of the experiment
subject	String	1		no	Name of the subject that was imaged
isSimulation	Int8	1		no	Flag indicating if the data in this file is simulated rather than measured

3.3 Tracer Parameters (group: /tracer/, optional)

Remarks: The tracer parameter group contains information about the MPI tracers used during the experiment. For each tracer its `name`, `batch`, `vendor`, `volume`, and molar `concentration` of `solute` per liter must be provided. Additionally, the time point of injection can be noted.

This version of the MDF can handle two basic scenarios. In the first one static tracer phantoms are used. In this case the phantom contains

A distinct tracers. These might be particles of different core sizes, mobile or immobilized particles for example. In this case `injectionTime` is not used. In the second case A boli (e.g. pulsed boli) are administrated during the measurement, in which case the approximate administration volume, tracer type and time point of injection can be provided. Note that the

injection clock recording the injection time should be synchronized with the clock, which provides the starting time of the measurement.

In case of a background measurement with no applied tracers in the scanner, the tracer group should be removed. Therefore, it is optional.

Parameter	Type	Dim	Unit/Format	Optional	Description
name	String	A		no	Name of tracer used in experiment
batch	String	A		no	Batch of tracer
vendor	String	A		no	Name of tracer supplier
volume	Float64	A	L	no	Total volume of applied tracer
concentration	Float64	A	mol(solute)/L	no	Molar concentration of solute per litre
solute	String	A		no	Solute, e.g. Fe
injectionTime	String	A	yyyy-mm-ddThh:mm:ss.ms	yes	UTC time at which tracer injection started

3.4 Scanner Parameters (group: /scanner/, non-optional)

Remarks: The scanner parameter group contains information about the the field **topology**, the **facility** where the scanner is installed and the MPI scanner used, such as the **name**, the **manufacturer**, the **boreSize**, **operator**.

Parameter	Type	Dim	Unit/Format	Optional	Description
name	String	1		no	Scanner name
facility	String	1		no	Facility where the MPI scanner is installed
operator	String	1		no	User who operates the MPI scanner
manufacturer	String	1		no	Scanner manufacturer
topology	String	1		no	Scanner topology (e.g. FFP, FFL, MPS)
boreSize	Float64	1	m	yes	Diameter of the bore

3.5 Acquisition Parameters (group: /acquisition/, non-optional)

Remarks: The acquisition parameter group can describe different imaging protocols and trajectory settings. The corresponding data is organized into general information within this group, a subgroup containing information on the D excitation channels and a subgroup containing information on the C receive channels.

In MPI a frame groups together all data used to reconstruct a single MPI image/tomogram. In the simplest scenario this data is acquired during one `/drivefield/period`. One may acquire as well several periods denoted by `numPeriods`. If averaging is applied the acquisition time

increases by `numAverages`. In a multi-patch setting J `offsetFields` or mechanical movements shift the gradient field by `offsetFieldShift` to different spatial positions, where J is the number of patches `numPatches` of a multi-patch measurement. At each position at least one full drive field cycle is used to acquire measurement data. Such a frame may consist of J sub-measurements, each of which is acquired and averaged over `numPeriods` and `numAverages` drive field cycles. For instance a Cartesian 2D trajectory with 100 lines could be realized by setting `numPatches` = 100.

Parameter	Type	Dim	Unit/Format	Optional	Description
<code>startTime</code>	String	1	yyyy-mm-ddThh:mm:ss.ms	no	UTC start time of MPI measurement
<code>framePeriod</code>	Float64	1	s	no	Time to complete a full frame (product of <code>/drivefield/period</code> , <code>numPeriods</code> , <code>numAverages</code> , and <code>numPatches</code>)
<code>numPeriods</code>	Integer	1	1	no	Number of drive-field periods per patch
<code>numAverages</code>	Integer	1	1	no	Number of block averages per patch
<code>numPatches</code>	Integer	1	1	no	Number of patches within a frame denoted by J
<code>numFrames</code>	Integer	1	1	no	Number of available measurement frames N
<code>gradient</code>	Float64	$J \times 3$	$\text{Tm}^{-1}\mu_0^{-1}$	yes	Gradient strength of the selection field in x , y , and z directions
<code>offsetField</code>	Float64	$J \times 3$	$\text{T}\mu_0^{-1}$	yes	Offset field applied for each patch in the measurement sequence
<code>offsetFieldShift</code>	Float64	$J \times 3$	m	yes	Position of the field free point (relative to origin/center)

3.5.1 Drive Field (group: `/acquisition/drivefield/`, non-optional)

Remarks: The drive field subgroup describes the excitation details of the imaging protocol. On the lowest level each MPI scanner contains D channels for excitation. Since most drive-field parameters may change from patch to patch they have a leading dimension J .

These excitation signals are usually sinusoidal and can be described by D amplitudes (drive field strengths), D phases, a base frequency, and D

dividers. In a more general setting generated drive-fields of channel d can be described by

$$H_d(t) = \sum_{l=1}^F A_l \Lambda_l(2\pi f_l t + \varphi_l)$$

where F is the number of frequencies on the channel, A_l is the drive-field strength, ϕ_l is the phase, f_l is the frequency (`baseFrequency/dividerl`),

and Λ_l is the waveform. The waveform is specified by a dedicated parameter **waveform**. it can be set to *sine*, *triangle* or *custom*. If set to *custom*, one can specify a custom waveform using the parameter **customWaveform**. The number of sampling points of the **customWaveform** is denoted by U . The triangle is defined to be a 2π periodization of the triangle function:

$$\Lambda_{\text{tri}}(t) = \left| t + \frac{\pi}{2} \right| - \frac{\pi}{2} \quad \text{for} \quad -\frac{3}{2}\pi \leq t \leq \frac{\pi}{2}$$

Parameter	Type	Dim	Unit/Format	Optional	Description
<code>numChannels</code>	Int64	1	1	no	Number of drive field channels, denoted by D
<code>strength</code>	Float64	$J \times D \times F$	$\text{T}\mu_0^{-1}$	no	Applied drive field strength
<code>phase</code>	Float64	$J \times D \times F$	rad, $[-\pi, \pi)$	no	Applied drive field phase φ
<code>baseFrequency</code>	Float64	1	Hz	no	Base frequency to derive drive field frequencies
<code>customWaveform</code>	Float64	$D \times F \times U$	1	yes	Custom waveform table
<code>divider</code>	Integer	$D \times F$	1	no	Divider of the baseFrequency to determine the drive field frequencies
<code>waveform</code>	String	$D \times F$	1	no	Waveform type: <i>sine</i> , <i>triangle</i> or <i>custom</i>
<code>period</code>	Float64	1	s	no	Trajectory period is determined by <code>lcm(divider)/baseFrequency</code>

3.5.2 Receiver (group: /acquisition/receiver/, non-optional)

Remarks: The receiver subgroup describes details on the MPI receiver. For a multi-patch sequence it is assumed, that signal acquisition only takes place during particle excitation. During each drive-field cycle, C receive channels record some quantity related to the magnetization dynamic. In most cases these will be voltage signals induced into the C receive coils, which are proportional to the change of the particle magnetization. The actual unit is denoted in `/measurement/unit`.

The MPI signal is acquired at V equidistant time points. Note that in most cases the signal is not measured directly at the receive coils but amplified and filtered first which may damp and distort the signal. A transfer function can optionally be stored in the parameter **transferFunction** which allows to calculate the magnetic moment out of the measured quantity. It is stored in frequency space representation where K is the number of discrete frequency components.

Parameter	Type	Dim	Unit/Format	Optional	Description
numChannels	Int64	1		no	Number of receive channels C
bandwidth	Float64	1	Hz	no	Bandwidth of the receiver unit
numSamplingPoints	Int64	1		no	Number of sampling points during one patch, denoted by V
transferFunction	Float64	$C \times K \times 2$	unit $\text{A}^{-1}\text{m}^{-2}$	yes	Transfer function of the receive channels in Fourier Domain. unit is the field from the <code>/measurement</code> group

3.6 Measurement (group: `/measurement/`, optional)

Remarks: MPI data is usually acquired by a series of measurements and optional background measurements. Here, we refer to background measurements as MPI data captured, when any signal generating material, e.g. a phantom or a delta sample is removed from the scanner bore. Initially, all data is available in time domain, where the data of a single frame consists of the signal recorded for all patches in each receive channel, i.e. $J \times C \times V$ data points per set with the temporal index being the fastest to access. If several measurements are acquired (indicated by `numFrames`), the frame dimension is the slowest to access. Along this dimension the frames are ordered with respect to the time at which they were acquired starting with the measurement acquired first and stopping with the measurement acquired last. We refer to this data as raw measurement data. In Fourier representation each frame would be stored by $J \times C \times K \times 2$ data points with the last dimension accounting for the complex data and $K = V/2 + 1$.

During a measurement, the analog signal is usually converted into $(r_1, \dots, r_{JV}) \in \mathbb{Z}^J \times \mathbb{Z}^V$ integer values for each channel $c \in C$ using analog to digital converters. Often this raw data is stored instead of the physical quantities they represent. To bring the raw values into a physical representation one can map $r_i \mapsto (a_c r_i + b_c)U$, where a_c and b_c are the characteristic dimensionless scaling factor and offset the receive channel $c \in C$ and U is the corresponding **unit**, i.e. usually Volt. Note that these factors are also used to map (unsigned) integers to a floating point range.

Often it is not convenient to store the raw data but to perform certain processing steps and store the processed data. These steps may lead to a reduction of the number of sampling points from V to W or a corresponding reduction of frequency components K depending on the final representation in which the raw/processed data is stored. The most common processing steps are:

1. spectral leakage correction which may be applied to ensure that each individual frame is periodic.
2. background correction, where the background signal is subtracted.
3. Fourier transformation bringing the data from time into the Fourier representation and storing them in Fourier representation.
4. transfer function correction to obtain the magnetic moment that has been measured.
5. frequency selection to reduce the number of frequency components, e.g. bandwidth reduction or selection of high signal frequency components.
6. dimension permutation which is usually applied to Fourier transformed data exchanging the storing order of the data for fast access to the frames.

7. frame permutation to reorder the frames within the data set.

For each of the steps above there is a corresponding flag within this group indicating if the corresponding processing step has been carried out.

During processing one might want to keep track which of the final N frames belong to background measurements and which do not. Therefore, the binary mask **isBackgroundFrame** can be used. If **isBackgroundFrame**

is not provided it is assumed that no background measurements are present. If frequency selection has been performed **frequencySelection** stores the K frequency components (subset) selected from the set of acquired frequency components. If performed, a frame permutation can be described by i.e. a bijective mapping $\sigma : \{1, 2, \dots, N\} \rightarrow \{1, 2, \dots, N\}$ of the set of frame indices to itself. If such a permutation is performed, σ is stored in the one-line notation as $\sigma(1), \sigma(2), \dots, \sigma(N)$ in **framePermutation**.

Parameter	Type	Dim	Optional	Description
<code>unit</code>	<code>String</code>	1	no	SI unit of the measured quantity, usually V
<code>dataConversionFactor</code>	<code>Number</code>	$C \times 2$	yes	Dimension less scaling factor and offset (a_c, b_c) to convert raw data into a physical quantity with corresponding unit of measurement <code>unit</code>
<code>data</code>	<code>Number</code>	$N \times J \times C \times K \times 2$ or $J \times C \times K \times N \times 2$ or $N \times J \times C \times W$ or $J \times C \times W \times N$	no	Processed data
<code>isBackgroundFrame</code>	<code>Int8</code>	N	yes	Mask indicating for each of the N frames if it is a background measurement (true) or not
<code>isSpectralLeakageCorrected</code>	<code>Int8</code>	1	no	Flag, if spectral leakage correction has been applied
<code>isBackgroundCorrected</code>	<code>Int8</code>	1	no	Flag, if the background has been subtracted
<code>isFourierTransformed</code>	<code>Int8</code>	1	no	Flag, if the data is stored in frequency space
<code>isTransferFunctionCorrected</code>	<code>Int8</code>	1	no	Flag, if the data has been corrected by the <code>transferFunction</code>
<code>isFrequencySelection</code>	<code>Int8</code>	1	no	Flag, if only a subset of frequencies has been selected and stored, see <code>frequencySelection</code>
<code>isPermuted</code>	<code>Int8</code>	1	no	Flag, if the frame dimension N has been moved to the last dimension (second last for complex data)
<code>isFramePermutation</code>	<code>Int8</code>	1	no	Flag, if the order of frames has been changed, see <code>framePermutation</code>
<code>frequencySelection</code>	<code>Integer</code>	K	<code>isFrequencySelection</code>	Indices of selected frequency components
<code>framePermutation</code>	<code>Integer</code>	N	<code>isFramePermutation</code>	Indices of original frame order

3.7 Calibration (group: /calibration/, optional)

Remarks: The calibration group describes a calibration measurement (system matrix), although it does not hold the data itself. Each of the measurements is taken with a calibration sample (delta sample) at a fixed position inside the FOV of the device. (If available, the background measurements are taken with the delta sample outside of the FOV of the scanner.) Usually, the calibration measurements are not stored as raw measurements but as processed data, where at least averaging, Fourier transformation, frame permutation and transposition of the data has been performed yielding N processed calibration frames. N includes the background measurements, whereas O is the number of calibrated spatial positions scans. Which steps have been performed is documented in `/measurement`.

If the measurements were taken on a regular grid of size $N_x \times N_y \times N_z$ the permutation is usually done such that measurements are ordered with respect to their x position first, second with respect to their y position and last with respect to their z position. Background measurements are collected at the end in `/measurement/data`, which in combination with reordering of the measurements allows fast access to the system matrix. If a different storage order is used this can be documented using the optional parameter `order`. For non-regular sampling points there is the possibility to explicitly store all O positions. In case of acquiring a hybrid system matrix, the spatial positions may be emulated by applying `offsetFields` to the measurement chamber.

Parameter	Type	Dim	Unit/Format	Optional	Description
<code>method</code>	String	1		no	Method used to obtain calibration data. Can for instance be robot, hybrid, or simulation
<code>size</code>	Integer	3		yes	Number of voxels in each dimension, inner product is O
<code>order</code>	String	1		yes	Ordering of the dimensions, default is xyz
<code>positions</code>	Float64	$O \times 3$	m	yes	Position of each of the grid points, stored as (x, y, z) triples
<code>offsetFields</code>	Float64	$O \times 3$	$T\mu_0^{-1}$	yes	Applied offset field strength to emulate a spatial position (x, y, z)
<code>deltaSampleSize</code>	Float64	3	m	yes	Size of the delta sample used for calibration scan
<code>fieldOfView</code>	Float64	3	m	yes	Field of view of the system matrix
<code>fieldOfViewCenter</code>	Float64	3	m	yes	Center of the system matrix (relative to origin/center)
<code>snr</code>	Float64	$J \times C \times K$		yes	Signal-to-noise estimate for recorded frequency components

3.8 Reconstruction Results (group: `/reconstruction/`, optional)

Reconstruction results are stored using the parameter **data** inside this group. **data** contains a $Q \times P \times S$ array, where Q denotes the number of reconstructed frames within the data set, P denotes the number of voxels and S the number of multispectral channels. If no multispectral reconstruction is performed then one may set $S = 1$. Depending on the reconstruction the grid of the reconstruction data can be different from the system matrix grid. Hence, grid parameters are mirrored in the **/reconstruction** group.

For analysis of the MPI tomograms it is often required to know which parts of the reconstructed tomogram have been covered by the trajectory of the field free region. In MPI one refers to the non-covered region as overscan region. Therefore, the optional field **isOverscanRegion** indicated for each voxel if it is part of the overscan region. If no voxel lies within the overscan region **isOverscanRegion** may be omitted.

Parameter	Type	Dim	Unit/Format	Optional	Description
data	Number	$Q \times P \times S$		no	Reconstructed data
size	Integer	3		yes	Number of voxels in each dimension, inner product is P
order	String	1		yes	Ordering of the dimensions, default is xyz
positions	Float64	$P \times 3$	m	yes	Position of each of the grid points, stored as (x, y, z) tripels
fieldOfView	Float64	3	m	yes	Field of view of reconstructed data
fieldOfViewCenter	Float64	3	m	yes	Center of the reconstructed data (relative to scanner origin/center)
isOverscanRegion	Int8	P		yes	Mask indicating for each of the P voxels if it is part of the overscan region (true) or not

4 Changelog

4.1 v2.0.0

- Updated Affiliations in the MDF specification.
- Made extensive improvements to the descriptions of fields and groups.
- In v1.x the MDF allowed many fields to have varying dimensions depending on the context. As of version 2.0.0 only one field offers this freedom. This change should make implementations handling MDF files less complex.
- Specified supported data types.
- Added table of all parameters in the MDF.
- Added section describing the possibility to add custom fields to MDF files.
- Added description for optional and non optional groups and conditional, optional, and non-optional data sets.
- Added short section on the code examples on the Github repository.
- Removed section on sanity check along side with sanity check.
- Rename `/date` to `/time` for consistency reasons.
- Remove `/study/reference` since this functionality is now covered by the integrated background measurements.
- Rename `/study/simulation` to `/study/isSimulation` for consistency reasons and changed type to `Int8`.
- Created new group `/experiment` with fields `/experiment/name`, `/experiment/number` and `/experiment/description` to be able to provide more fine grained information on study and experiment.
- Moved `/study/subject` and `/study/isSimulation` to `/experiment/subject` and `/experiment/isSimulation`.
- Renamed `/tracer/time` to `/tracer/injectionTime`.
- Added the possibility store the tracer concentration also for non iron based tracer materials by adding the `/tracer/solute` field and re-defining the field `tracer/concentration`.
- Renamed field `/tracer/time` to `/tracer/injectionTime` to be more specific.
- Added the dimension `A` to all fields of the `tracer` group to be able to describe settings where multiple tracers are used or tracers are administered multiple times.
- Added field `/scanner/boreSize` to describe the scanner.
- Set all fields but `topology` in the `/scanner` group to be optional.
- Rename `/acquisition/time` to `/acquisition/startTime`.
- `/acquisition/gradient` is now optional since it is now mandatory for MPS measurements.
- Added `/acquisition/offsetField` and `/acquisition/offsetFieldShift` to describe homogeneous offset fields.
- Support for triangle wave forms and fully arbitrary excitation waveforms has been added by adding the fields `/drivefield/phase`, `/drivefield/customWaveform`, `/drivefield/waveform`.
- Support for multiple excitation frequencies on a drive-field channel has been added by introducing a new dimension `F` to the fields `/drivefield/strength`, `/drivefield/phase`, `/drivefield/customWaveform`, `/drivefield/waveform`, and `/drivefield/divider`.

- Removed `fieldOfView` and `fieldOfViewCenter` from `/drivefield` group. `/acquisition/offsetField` and `/acquisition/offsetFieldShift` replace `fieldOfViewCenter`. The `fieldOfView` can be derived from the gradient strength and drive field strength.
- Moved `/drivefield/averages` to `/receiver/numAverages`
- Remove `/acquisition/receiver/frequencies` since it can be directly derived from `/acquisition/receiver/bandwidth` and `/acquisition/receiver/numSamplingPoints`.
- **TODO Tobi: record changes to `/measurement` group here.** Added possibility to store the transformation from raw data to a physical representation with units. Signal to noise ratios can now be stored for each patch individually. To do so the dimension P was added to this field.
- **TODO Tobi: record changes to `/calibration` group here.**
- Added possibility to mark the overscan region.
- Added new section changelog to the MDF documentation to record the development of the MDF.
- Updated `README.md` on the github repository.

4.2 v1.0.5

- Added the possibility to store different channels of reconstructed data.
- Added support for receive channels with different characteristics (e.g. bandwidth).
- Made dataset `/acquisition/receiver/frequencies` optional.
- Extended the description on the data types, which are used to store data.

- Added references for Julia and HDF5 to the specifications.

4.3 v1.0.4

- Clarify that HDF5 datasets are used to store MPI parameters.

4.4 v1.0.3

- Updated Affiliations in the MDF specification.
- Included data download into the Python and Matlab example code.
- Changes in the Python and Matlab example code to be better comparable to the Julia example code.

4.5 v1.0.2

- Added reference to arXiv paper and bibtex file for reference.

4.6 v1.0.1

- A sanity check within the Julia code shipped alongside the specifications.
- An update to the specification documenting the availability of a sanity check.
- Updated MDF files on <https://www.tuhh.de/ibi/research/mpi-data-format.html>.
- Updated documentation to the Julia, Matlab and Python reconstruction scripts.
- Improved Julia reconstruction script, automatically downloading the required MDF files.

References

- [1] Jeff Bezanson, Stefan Karpinski, Viral B. Shah, and Alan Edelman. Julia: A fast dynamic language for technical computing. *CoRR*, abs/1209.5145, 2012.
- [2] Jeff Bezanson, Jiahao Chen, Stefan Karpinski, Viral B. Shah, and Alan Edelman. Array operators using multiple dispatch: a design methodology for array implementations in dynamic languages. *CoRR*, abs/1407.3845, 2014.
- [3] Jeff Bezanson, Alan Edelman, Stefan Karpinski, and Viral B. Shah. Julia: A fresh approach to numerical computing. *CoRR*, abs/1411.1607, 2014.
- [4] The HDF Group. Hierarchical Data Format, version 5, 1997-2016. <http://www.hdfgroup.org/HDF5/>.
- [5] Paul J Leach, Michael Mealling, and Rich Salz. A universally unique identifier (uuid) urn namespace. 2005.
- [6] Bernhard Gleich and Jürgen Weizenecker. Tomographic imaging using the nonlinear response of magnetic particles. *Nature*, 435(7046):1214–1217, 2005.